

AN 2002:214480 CAPLUS  
 DN 136:377729  
 TI Novel high birefringence dibenzothiophenylacetylene liquid crystals  
 AU Sekine, Chizu; Ishitobi, Masamitsu; Iwakura, Kazunori; Minai, Masayoshi;  
 Fujisawa, Koichi  
 CS Tsukuba Research Laboratory, Sumitomo Chemical Co. Ltd., Tsukuba,  
 300-3294, Japan  
 SO Liquid Crystals (2002), 29(3), 355-367  
 CODEN: LICRE6; ISSN: 0267-8292  
 PB Taylor & Francis Ltd.  
 DT Journal  
 LA English  
 CC 75-11 (Crystallography and Liquid Crystals)  
 Section cross-reference(s): 27, 73, 74  
 AB The authors have designed, synthesized and evaluated  
 dibenzothiophenylacetylene homologs as new heterocyclic mols. which were  
 expected to have high .DELTA..alpha. values and short wavelength UV  
 absorption spectra. The dibenzothiophenyl acetylene homologs exhibited  
 wide nematic phase ranges and had very high extrapolated .DELTA.n of over  
 0.6 and directly measured values of 0.5. The compds. with two  
 dibenzothiophenyl rings were colorless, so that the authors have succeeded  
 in obtaining colorless super-high .DELTA.n liq. crystals. The authors  
 also analyzed the contribution of the transition band to the refractive  
 indexes and the birefringence. From the anal., the main origins of  
 .DELTA.n for compds. 1 and 2 are lower MOs than the HOMO and this results  
 in the compatibility of large .DELTA.n and lack of color. The  
 dibenzothiophenylacetylene compds. behaved according to the authors'  
 design expectations.  
 ST birefringence dibenzothiophenylacetylene deriv liq crystal prepn property  
 IT Liquid crystals  
 (design, synthesis, and mesomorphic and optical properties of  
 high-birefringence dibenzothiophenylacetylene derivs.)  
 IT Birefringence  
 UV and visible spectra  
 (of dibenzothiophenylacetylene deriv. liq. crystals)  
 IT Polarizability  
 Refractive index  
 (of high-birefringence dibenzothiophenylacetylene derivs.)  
 IT Liquid crystals  
 (transitions; of high-birefringence dibenzothiophenylacetylene derivs.)  
 IT 425404-03-1P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (prepn. and (hexylidene)dibenzothiophenylacetylene)  
 IT 25288-76-0P, 3-Dibenzothiophenamine  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (prepn. and bromination of)  
 IT 425404-07-5P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (prepn. and desilylation of)  
 IT 425404-00-8P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (prepn. and esterification of)  
 IT 1013-23-6P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (prepn. and nitric acid reaction with)  
 IT 425403-99-2P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (prepn. and oxidn. of)

IT 425403-94-7P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (prepn. and reaction dibenzothiophenylacetylene(ethylphenyl  
 trifluorosulfonate))

IT 425403-93-6P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (prepn. and reaction potassium hydroxide in toluene)

IT 425403-96-9P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (prepn. and reaction with dibenzothiophenylacetylene and  
 pentyloxyphenylacetylene)

IT 425404-04-2P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (prepn. and reaction with hexyne and phenyldioxoborane)

IT 425403-97-0P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (prepn. and reaction with nitric acid)

IT 425404-08-6P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (prepn. and reaction with pentyloxydibenzothiophenylacetylene(ethylphen  
 yl trifluorosulfonate))

IT 97511-04-1P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (prepn. and reaction with propargyl alc. in presence of palladium  
 dichloride, triphenylphosphine and triethylamine in Et acetate)

IT 425404-01-9P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (prepn. and reaction with triethylamine and toluenesulfonic acid in  
 methanol)

IT 425403-95-8P 425404-02-0P 425404-05-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (prepn. and reaction with trifluoromethanesulfonic anhydride)

IT 425404-06-4P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (prepn. and reaction with trimethylsilylacetylene)

IT 68925-98-4P 425403-98-1P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (prepn. and redn. of)

IT 425403-90-3P 425403-91-4P 425403-92-5P  
 RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP  
 (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC  
 (Process)  
 (prepn., liq. crystal properties and optical properties of)

IT 67589-39-3, 4-Ethoxyphenyl trans-4-propylcyclohexylcarboxylate  
 67589-41-7, 4-Butoxyphenyl trans-4-propylcyclohexylcarboxylate  
 67589-47-3, 4-Ethoxyphenyl trans-4-butylcyclohexylcarboxylate  
 67589-52-0, 4-Methoxyphenyl trans-4-pentylcyclohexylcarboxylate  
 67589-53-1, 4-Ethoxyphenyl trans-4-pentylcyclohexylcarboxylate  
 RL: NUU (Other use, unclassified); PRP (Properties); USES (Uses)  
 (refractive indexes and dichroic ratios of polarized UV spectra of  
 dibenzothiophenylacetylene derivs. in liq. crystal mixt. contg.)

RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 RE

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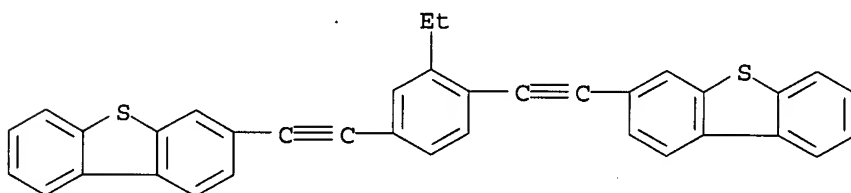
IT 425403-90-3P 425403-91-4P 425403-92-5P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)

(prepn., liq. crystal properties and optical properties of)

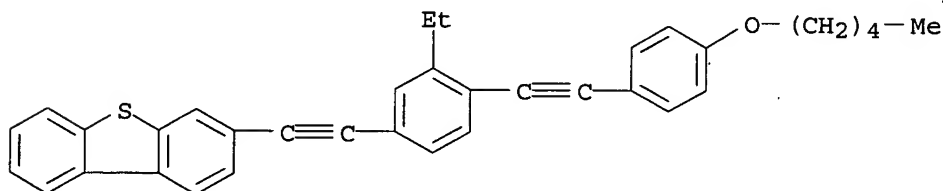
RN 425403-90-3 CAPLUS

CN Dibenzothiophene, 3,3'-[(2-ethyl-1,4-phenylene)di-2,1-ethynediyl]bis-(9CI) (CA INDEX NAME)



RN 425403-91-4 CAPLUS

CN Dibenzothiophene, 3-[[3-ethyl-4-[[4-(pentyloxy)phenyl]ethynyl]phenyl]ethynyl]- (9CI) (CA INDEX NAME)

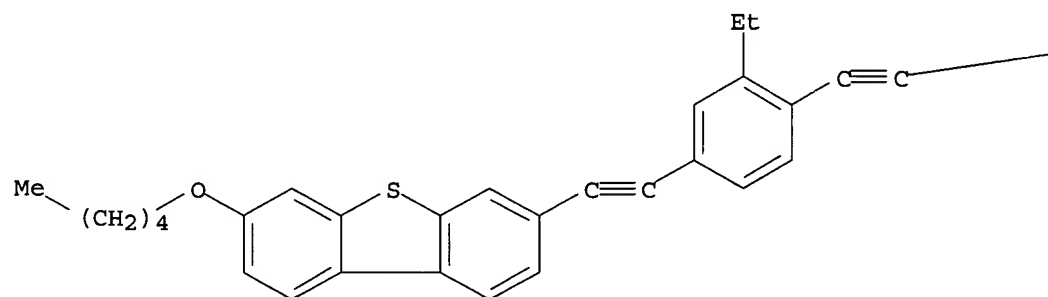


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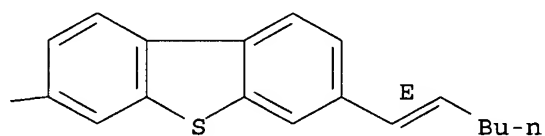
CN Dibenzothiophene, 3-[[3-ethyl-4-[[7-(1E)-1-hexenyl-3-dibenzothiophenyl]ethynyl]phenyl]ethynyl]-7-(pentyloxy)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

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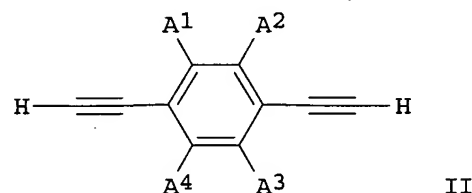
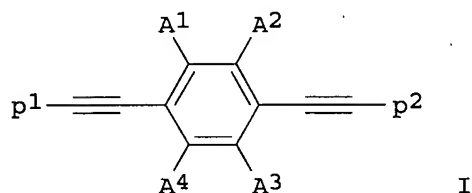
PAGE 1-B



AN 2002:616226 CAPLUS  
 DN 137:177210  
 TI Compound having phenylacetylene structure, liquid crystal composition, polymer, optically anisotropic product, optical or liquid crystal element, dibenzothiophene compound, intermediate, and process for producing the same  
 IN Sekine, Chizu; Ishitobi, Masamitsu; Fujisawa, Koichi; Iwakura, Kazunori; Minai, Masayoshi  
 PA Japan  
 SO U.S. Pat. Appl. Publ., 74 pp.  
 CODEN: USXXCO  
 DT Patent  
 LA English  
 IC ICM C09K019-52  
 ICS C09K019-30; C07C025-13; C07D495-00; C07D335-10  
 NCL 428001100  
 CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)  
 Section cross-reference(s): 75

FAN.CNT 1

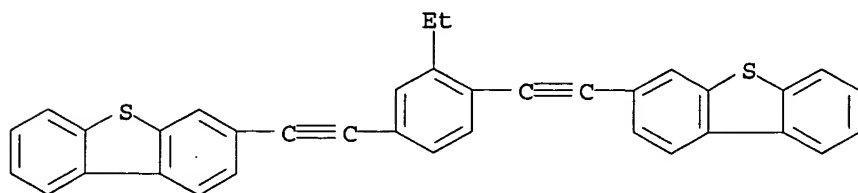
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2002110650	A1	20020815	US 2002-67871	20020208
	JP 2002255960	A2	20020911	JP 2001-52954	20010227
	JP 2002322174	A2	20021108	JP 2002-24353	20020131
	JP 2002322215	A2	20021108	JP 2002-24425	20020131
	GB 2380192	A1	20030402	GB 2002-2907	20020207
	DE 10205367	A1	20021212	DE 2002-10205367	20020208
PRAI	JP 2001-33782	A	20010209		
	JP 2001-37311	A	20010214		
	JP 2001-52954	A	20010227		
OS	MARPAT 137:177210				
GI					



AB The present invention relates to liq. crystal compns., polymers, optically anisotropic products, and optical or liq. crystal elements that have large refractive index anisotropy, mix easily with other liq. crystals, have advantageous stability against light, and exhibit absorption at practically short wavelength in the UV region. The present invention also relates to phenylacetylene structure compds. which are useful as optical display, and recording materials, as optical compensators, polarizer materials, reflector plates, etc., all for liq. crystal display devices. The compds. are represented by I (A1-4 = H, F, C1-10 alkyl or alkoxy

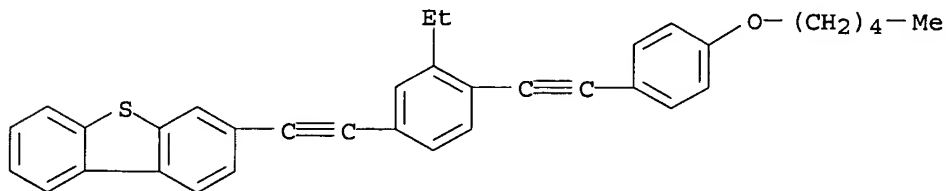
optionally substituted with F; P1,2 = structure fulfilling the conditions of HOMO energy and polarizability) and have a phenylacetylene structure, wherein difference .DELTA.E in energy of HOMO of parts II, P1-H and P2-H calcd. by the method of MOs is .gtoreq. 0.3 eV, and the polarizability anisotropy .DELTA..alpha. of a mol. represented by I calcd. in the same way is .gtoreq. 500 A.U.

- ST liq crystal display phenylacetylene dibenzothiophene compd  
IT Liquid crystal displays  
(Compd. having phenylacetylene structure and dibenzothiophene compd.  
for liq. crystal compn. for)
- IT **425403-90-3P 425403-91-4P 446023-58-1P**  
RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or  
engineered material use); PREP (Preparation); USES (Uses)  
(compd. having phenylacetylene structure and dibenzothiophene compd.  
for liq. crystal display)
- IT 379268-41-4P  
RL: SPN (Synthetic preparation); TEM (Technical or engineered material  
use); PREP (Preparation); USES (Uses)  
(compd. having phenylacetylene structure and dibenzothiophene compd.  
for liq. crystal display)
- IT 224648-09-3 239104-43-9 239104-50-8 251467-52-4 296255-72-6  
299411-32-8 299411-39-5 446023-47-8 446023-48-9  
RL: TEM (Technical or engineered material use); USES (Uses)  
(liq. crystal compn.; compd. having phenylacetylene structure and  
dibenzothiophene compd. for liq. crystal display)
- IT 425403-94-7P 425403-96-9P 425404-00-8P 425404-01-9P 425404-03-1P  
446023-43-4P 446023-45-6P  
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation); RACT (Reactant or reagent)  
(prepn. of compd. having phenylacetylene structure and dibenzothiophene  
compd. for liq. crystal display)
- IT **446023-46-7P**  
RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or  
engineered material use); PREP (Preparation); USES (Uses)  
(prepn. of compd. having phenylacetylene structure and dibenzothiophene  
compd. for liq. crystal display)
- IT 110-87-2, Dihydropyran 115-19-5, 2-Methyl-3-butyne-2-ol 132-65-0,  
Dibenzothiophene 274-07-7, Catecholborane 628-17-1, 1-Iodopentane  
693-02-7, 1-Hexyne 814-68-6, Acrylic acid chloride 4286-55-9  
50816-19-8, 8-Bromo-octanol 79887-16-4 350036-14-5  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(prepn. of compd. having phenylacetylene structure and dibenzothiophene  
compd. for liq. crystal display)
- IT 1013-23-6P 25288-76-0P, 3-Dibenzothiophenamine 56554-20-2P  
68925-98-4P 97511-04-1P 425403-95-8P 425403-97-0P 425403-98-1P  
425403-99-2P 425404-02-0P 425404-04-2P 446023-40-1P 446023-41-2P  
446023-42-3P 446023-44-5P 446023-49-0P 446023-50-3P 446023-51-4P  
446023-52-5P 446023-53-6P 446023-54-7P 446023-55-8P  
**446023-56-9P 446023-57-0P**  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(prepn. of compd. having phenylacetylene structure and dibenzothiophene  
compd. for liq. crystal display)
- IT **425403-90-3P 425403-91-4P 446023-58-1P**  
RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or  
engineered material use); PREP (Preparation); USES (Uses)  
(compd. having phenylacetylene structure and dibenzothiophene compd.  
for liq. crystal display)
- RN 425403-90-3 CAPLUS  
CN Dibenzothiophene, 3,3'-[(2-ethyl-1,4-phenylene)di-2,1-ethynediyl]bis-  
(9CI) (CA INDEX NAME)



RN 425403-91-4 CAPLUS

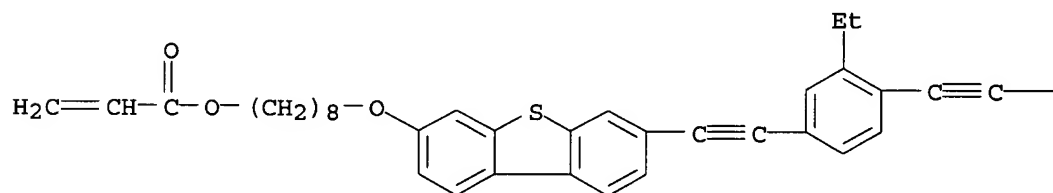
CN Dibenzothiophene, 3-[[3-ethyl-4-[[4-(pentyloxy)phenyl]ethynyl]phenyl]ethynyl]- (9CI) (CA INDEX NAME)



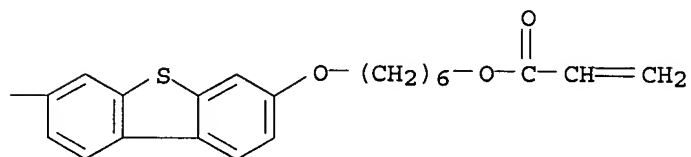
RN 446023-58-1 CAPLUS

CN 2-Propenoic acid, 8-[[7-[[3-ethyl-4-[[7-[[6-[[1-oxo-2-propenyl]oxy]hexyl]oxy]-3-dibenzothiényl]ethynyl]phenyl]ethynyl]-3-dibenzothiényl]oxy]octyl ester (9CI) (CA INDEX NAME)

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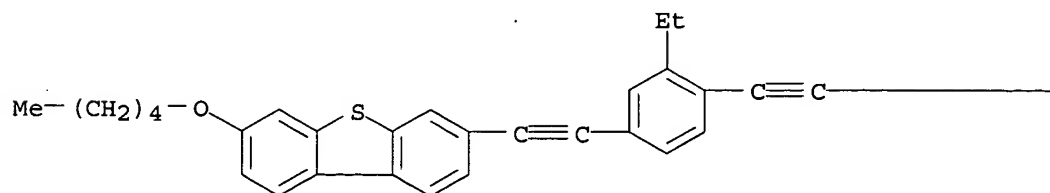
IT 446023-46-7P

RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)  
(prepn. of compd. having phenylacetylene structure and dibenzothiophene compd. for liq. crystal display)

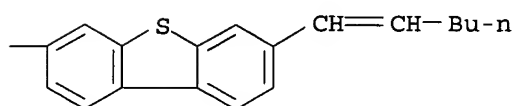
RN 446023-46-7 CAPLUS

CN Dibenzothiophene, 3-[[3-ethyl-4-[[7-(1-hexenyl)-3-dibenzothiényl]ethynyl]phenyl]ethynyl]-7-(pentyloxy)- (9CI) (CA INDEX NAME)

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IT 446023-56-9P 446023-57-0P

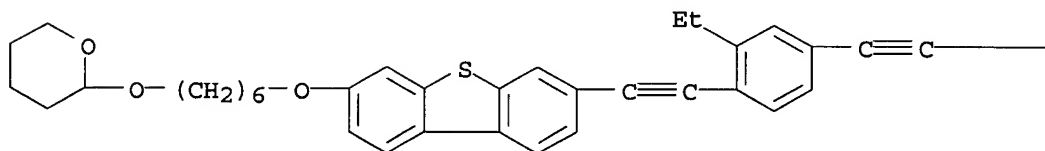
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of compd. having phenylacetylene structure and dibenzothiophene compd. for liq. crystal display)

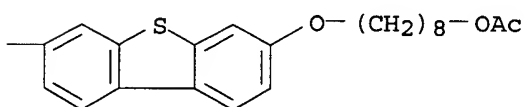
RN 446023-56-9 CAPLUS

CN 1-Octanol, 8-[[7-[[3-ethyl-4-[[7-[[6-[(tetrahydro-2H-pyran-2-yl)oxy]hexyl]oxy]-3-dibenzothiophenyl]ethynyl]phenyl]ethynyl]-3-dibenzothiophenyl]oxy]-, acetate (9CI) (CA INDEX NAME)

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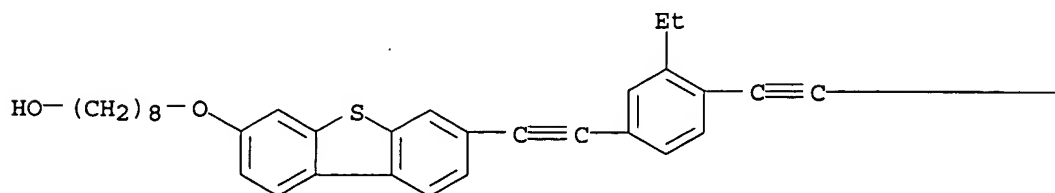
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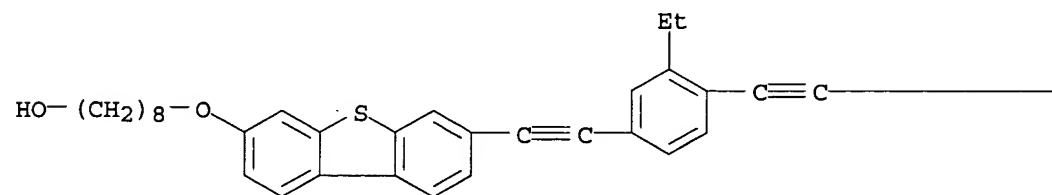
CN 1-Octanol, 8-[[7-[[3-ethyl-4-[[7-[[6-(6-hydroxyhexyl)oxy]-3-dibenzothiophenyl]ethynyl]phenyl]ethynyl]-3-dibenzothiophenyl]oxy]- (9CI) (CA INDEX NAME)

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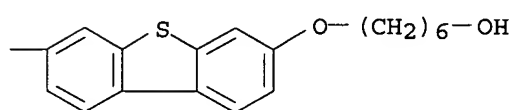


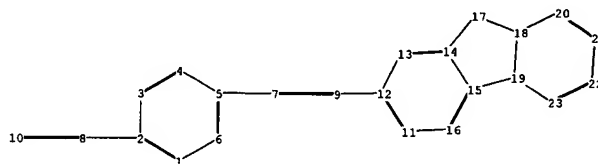
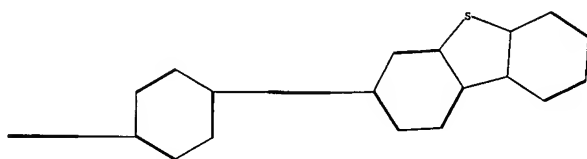


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PAGE 1-B





chain nodes :

7 8 9 10

ring nodes :

1 2 3 4 5 6 11 12 13 14 15 16 17 18 19 20 21 22 23

chain bonds :

2-8 5-7 7-9 8-10 9-12

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 14-17 15-16 15-19  
17-18 18-19 18-20 19-23 20-21 21-22 22-23

exact/norm bonds :

14-17 15-19 17-18 18-19 18-20 19-23 20-21 21-22 22-23

exact bonds :

2-8 5-7 7-9 8-10 9-12

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS  
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom  
21:Atom 22:Atom 23:Atom